

*Pnma*

$D_{2h}^{16}$

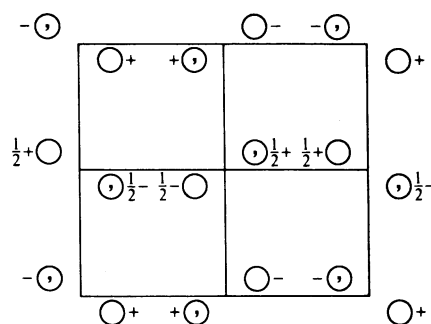
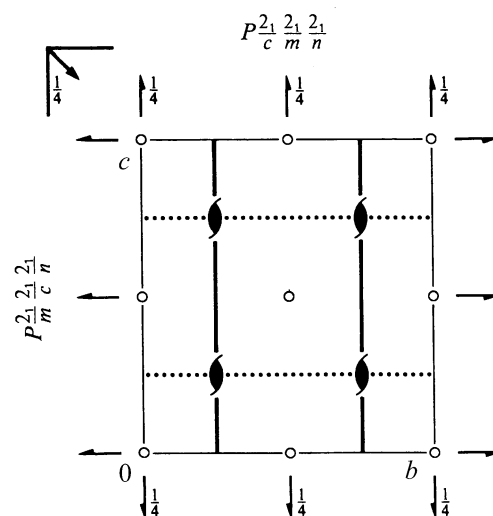
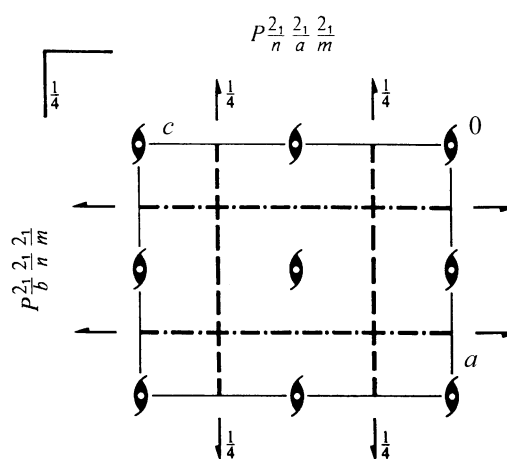
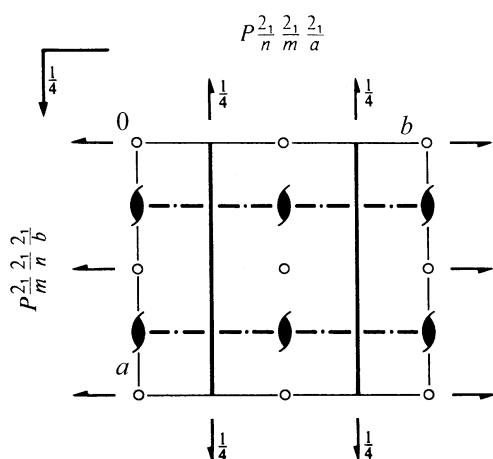
*mmm*

Orthorhombic

No. 62

$P 2_1/n 2_1/m 2_1/a$

Patterson symmetry *Pmmm*



Origin at  $\bar{1}$  on 12, 1

Asymmetric unit  $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{4}; 0 \leq z \leq 1$

Symmetry operations

- |                         |  |                                      |  |
|-------------------------|--|--------------------------------------|--|
| (1) 1                   | (2) $2(0, 0, \frac{1}{2})$ $\frac{1}{4}, 0, z$ | (3) $2(0, \frac{1}{2}, 0)$ $0, y, 0$ | (4) $2(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, \frac{1}{4}$ |
| (5) $\bar{1}$ $0, 0, 0$ | (6) $a$ $x, y, \frac{1}{4}$                    | (7) $m$ $x, \frac{1}{4}, z$          | (8) $n(0, \frac{1}{2}, \frac{1}{2})$ $\frac{1}{4}, y, z$ |

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2); (3); (5)

**Positions**

		Coordinates				Reflection conditions
Multiplicity, Wyckoff letter, Site symmetry						General:
8	<i>d</i> 1	(1) $x, y, z$ (5) $\bar{x}, \bar{y}, \bar{z}$	(2) $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ (6) $x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$	(3) $\bar{x}, y + \frac{1}{2}, \bar{z}$ (7) $x, \bar{y} + \frac{1}{2}, z$	(4) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (8) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$	$0kl: k + l = 2n$ $hk0: h = 2n$ $h00: h = 2n$ $0k0: k = 2n$ $00l: l = 2n$
4	<i>c</i> . <i>m</i> .	$x, \frac{1}{4}, z$	$\bar{x} + \frac{1}{2}, \frac{3}{4}, z + \frac{1}{2}$	$\bar{x}, \frac{3}{4}, \bar{z}$	$x + \frac{1}{2}, \frac{1}{4}, \bar{z} + \frac{1}{2}$	Special: as above, plus no extra conditions
4	<i>b</i> $\bar{1}$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	$hkl: h + l, k = 2n$
4	<i>a</i> $\bar{1}$	$0, 0, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl: h + l, k = 2n$

**Symmetry of special projections**

Along [001]  $p2gm$   
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$     $\mathbf{b}' = \mathbf{b}$   
 Origin at  $0, 0, z$

Along [100]  $c2mm$   
 $\mathbf{a}' = \mathbf{b}$     $\mathbf{b}' = \mathbf{c}$   
 Origin at  $x, \frac{1}{4}, \frac{1}{4}$

Along [010]  $p2gg$   
 $\mathbf{a}' = \mathbf{c}$     $\mathbf{b}' = \mathbf{a}$   
 Origin at  $0, y, 0$